Conventions, Accuracy Metrics, Classification, Regression

Nipun Batra

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Outline

Introduction and Demos

Machine Learning Fundamentals

First ML Example: Tomato Quality Prediction

Classification vs Regression

Classification Metrics

Regression Metrics

Data Visualization and Baselines

Summary and Key Takeaways

Introduction and Demos

Demo

• Complete PoseNet Demo

Demo

- Complete PoseNet Demo
- Blog post from Google

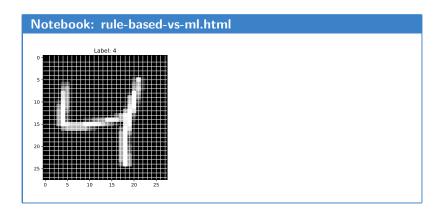
Demo

- Complete PoseNet Demo
- Blog post from Google
- Rock Paper Scissors

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Let us work on the digit recognition problem.



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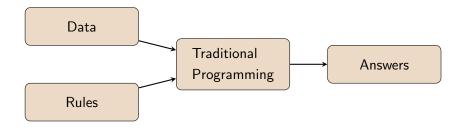
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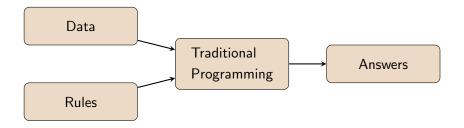
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- There can be some cases of 4 where the width of each stroke is different

Machine Learning Fundamentals

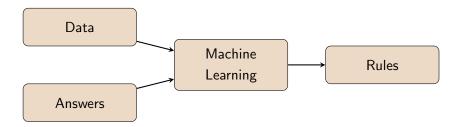
Traditional Programming vs Machine Learning



Traditional Programming



Machine Learning



"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P if its performance at tasks in T, as measured by P, improves with experience E." - Tom Mitchell

First ML Example: Tomato Quality Prediction

Quick Question!

In machine learning, which of the following is typically NOT a useful feature?

• a) Color of a tomato for quality prediction

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- a) Color of a tomato for quality prediction
- b) Size of a house for price prediction

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In machine learning, which of the following is typically NOT a useful feature?

- a) Color of a tomato for quality prediction
- b) Size of a house for price prediction
- c) Sample ID number
- d) Age for medical diagnosis

Answer: c) Sample ID numbers are arbitrary identifiers, not meaningful features!

First ML Task: Grocery Store Tomato Quality Prediction

Problem statement: You want to predict the quality of a tomato given its visual features.

Dataset

Imagine you have some past data on quality of tomatoes. What visual features do you think will be useful?

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• Size

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- Size
- Colour

Imagine you have some past data on quality of tomatoes. What visual features do you think will be useful?

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Imagine you have some past data on quality of tomatoes. What visual features do you think will be useful?

- Size
- Colour
- Texture

Sample Dataset

Here is our example dataset with tomato features:

Sample	Colour	Size	Texture	Condition
1	Orange	Small	Smooth	Good
2	Red	Small	Rough	Good
3	Orange	Medium	Smooth	Bad
4	Yellow	Large	Smooth	Bad

Useful Features

Is the sample number a useful feature for predicting quality of a tomato?

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Answer: Usually no! Sample numbers are typically arbitrary identifiers and not meaningful features. Let us remove it.

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Let us modify our data table for now.

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad

Colour	Size	Texture	Condition
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- 2. Output or Response Variable

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1. Feature matrix $(\mathbf{X} \in \mathbb{R}^{n \times d})$ containing data of n samples each of which is d dimensional.

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- 2. Output vector $(\mathbf{y} \in \mathbb{R}^n)$ containing output variable for n samples.

• Feature matrix:
$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{bmatrix}$$
 where $\mathbf{x}_i \in \mathbb{R}^d$

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• Example (after encoding): $\mathbf{x}_1 = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$ (Orange=1, Small=0, Smooth=1)

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- Example (after encoding): $\mathbf{x}_1 = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$ (Orange=1, Small=0, Smooth=1)
- Complete dataset: $\mathcal{D} = \{(\mathbf{x}_i^\top, y_i)\}_{i=1}^n$

Estimate condition for unseen tomatoes (#5, 6) based on data set.

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad
Red	Large	Rough	?
Orange	Large	Rough	?

Testing Set

Testing set is similar to training set, but, does not contain labels for output variable.

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
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- 3. To Predict the condition for the Testing set

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- Q: Is predicting on test set enough to say our model generalises?
- A: Ideally, no!
- Ideally we want to predict "well" on all possible inputs. But, can we test that?
- No! Since, the test set is only a sample from all possible inputs.

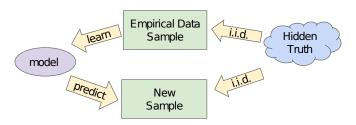


Image courtesy Google ML crash course

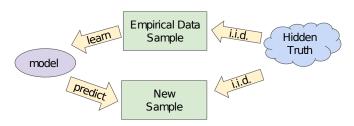


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Both the training set and the test set are samples drawn from the hidden true distribution (also sometimes called population)

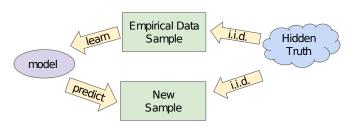


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More discussion later once we study bias and variance

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# People	Temp (C)	Energy (kWh)
4000	30	30
4200	30	32
4200	35	40
3000	20	?
1000	45	?

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Which of these is a regression problem?

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Answer: c) House prices are continuous values - that's regression!

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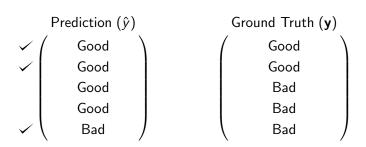
Classification Metrics

Metrics for Classification

Ground Truth: From the actual training set

Prediction: Made by the model

Accuracy



Accuracy

Prediction
$$(\hat{y})$$
 Ground Truth (\mathbf{y})
 \checkmark Good
Good
Good
Good
Good
Bad
Bad
Bad
Bad

$$\begin{aligned} \mathsf{Accuracy} &= \frac{|\{i: y_i = \hat{y}_i\}|}{n} \\ &= \frac{3}{5} = 0.6 \end{aligned}$$

- Set cardinality notation: $|\{i: y_i = \hat{y}_i\}|$
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- Alternative: Indicator function notation

Accuracy =
$$\frac{\sum_{i=1}^{n} \mathbf{1}[y_i = \hat{y}_i]}{n}$$

$$\text{where } \mathbf{1}[\text{condition}] = \begin{cases} 1 & \text{if condition is true} \\ 0 & \text{if condition is false} \end{cases}$$

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 Both notations are mathematically equivalent and commonly used in ML literature

$$\begin{array}{c} 1 \; \mathsf{sample} \; \{ \; \left(\begin{array}{c} \mathsf{Bad} \\ \mathsf{Good} \\ \mathsf{Good} \\ \\ \ldots \\ \mathsf{Good} \end{array} \right) \end{array}$$

Imbalanced Classes

$$\begin{array}{c} \text{1 sample } \{ \left(\begin{array}{c} \mathsf{Bad} \\ \mathsf{Good} \\ \mathsf{Good} \\ \\ \cdots \\ \mathsf{Good} \end{array} \right) \\ \text{Imbalanced Classes} \end{array}$$

Cases for this:

Cancer Screening

$$\begin{array}{c} \text{1 sample } \{ \left(\begin{array}{c} \mathsf{Bad} \\ \mathsf{Good} \\ \mathsf{Good} \\ \cdots \\ \mathsf{Good} \end{array} \right) \end{array}$$

Imbalanced Classes

Cases for this:

- Cancer Screening
- Planet Detection

Accuracy Metrics: Precision

Precision =
$$\frac{|\{i : y_i = \hat{y}_i = \text{Good}\}|}{|\{i : \hat{y}_i = \text{Good}\}|} = \frac{2}{4} = 0.5$$

"the fraction of relevant instances among the retrieved instances", i.e. "out of the number of times we predict Good, how many times is the condition actually Good"

Accuracy Metrics: Precision

$$\begin{array}{c} \text{Prediction } (\hat{y}) & \text{Ground Truth } (\mathbf{y}) \\ \rightarrow \checkmark & \text{Good} \\ \rightarrow \checkmark & \text{Good} \\ \rightarrow & \text{Good} \\ \rightarrow & \text{Good} \\ & \text{Bad} \\ & \text{Bad} \\ & \text{Good} \\ \end{array}$$

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"the fraction of relevant instances among the retrieved instances", i.e. "out of the number of times we predict Good, how many times is the condition actually Good"

Accuracy Metrics: Recall

Recall =
$$\frac{|\{i : y_i = \hat{y}_i = \text{Good}\}|}{|\{i : y_i = \text{Good}\}|} = \frac{2}{3} = 0.67$$

"the fraction of the total amount of relevant instances that were actually retrieved"

Quick Question!

In a dataset of 1000 samples where only 10 are positive cases, what's the accuracy of a classifier that always predicts "negative"?

• a) 1%

Quick Question!

- a) 1%
- b) 50%

Quick Question!

- a) 1%
- b) 50%
- c) 90%

Quick Question!

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- c) 90%
- d) 99%

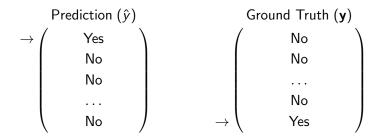
Quick Question!

In a dataset of 1000 samples where only 10 are positive cases, what's the accuracy of a classifier that always predicts "negative"?

- a) 1%
- b) 50%
- c) 90%
- d) 99%

Answer: d) 99% - but this classifier is useless! This shows why accuracy can be misleading.

Given predictions of whether a tissue is cancerous or not (n = 100).



Given predictions of whether a tissue is cancerous or not (n = 100).

$$\mbox{Accuracy} = \frac{98}{100} = 0.98 \qquad \qquad \mbox{Recall} = \frac{0}{1} = 0$$

$$\mbox{Precision} = \frac{0}{1} = 0$$

Accuracy Metrics: Confusion Matrix

		Ground Truth	
		Yes	No
Legicted	Yes	0	1
	No	1	98
L			

		Ground Truth	
		Yes	No
ָרָבְּרָ מַ	Yes	0	1
ובחורובת	No	1	98
L			

		Ground Truth	
		Yes	No
ted	Yes	True Positive	False Positive
redicted	No	False Negative	True Negative
Δ.			

		Ground Truth	
		Yes	No
redicted	Yes	True Positive	False Positive
redi	No	False Negative	True Negative
Д			

$$\mathsf{Precision} = \tfrac{\mathsf{TP}}{\mathsf{TP} + \mathsf{FP}}$$

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Δ.			

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$$\mathsf{Recall} = \tfrac{\mathsf{TP}}{\mathsf{TP} + \mathsf{FN}}$$

		Ground Truth	
		Yes	No
redicted	Yes	True Positive	False Positive
redi	No	False Negative	True Negative
Д			

$$\mathsf{Recall} = \tfrac{\mathsf{TP}}{\mathsf{TP} + \mathsf{FN}}$$

Accuracy Metrics: F-Score

		Ground Truth	
		Yes	No
ted	Yes	True Positive	False Positive
redicted	No	False Negative	True Negative
Д			

$$F-$$
 Score $=\frac{2\times$ Precision \times Recall Precision + Recall

Accuracy Metrics: Matthew's Correlation Coefficient

		Ground Truth		
		Yes	No	
ted	Yes	True Positive	False Positive	
redicted	No	False Negative	True Negative	
ص ٔ				

$$\frac{\text{TP} \times \text{TN} - \text{FP} \times \text{FN}}{\sqrt{(\text{TP} + \text{FP})(\text{TP} + \text{FN})(\text{TN} + \text{FP})(\text{TN} + \text{FN})}}$$

Accuracy Metrics: Example

For the data given below, calculate:

$$\begin{array}{ccc} & \text{G.T. Positive} & \text{G.T. Negative} \\ \text{Pred Positive} \left(& 90 & 4 \\ \text{Pred Negative} \left(& 1 & 1 \\ \end{array} \right) \end{array}$$

```
Precision = ?

Recall = ?

F-Score = ?

Matthew's Coeff. = ?
```

Accuracy Metrics: Answer

For the same data

G.T. Positive G.T. Negative Pred Positive
$$\begin{pmatrix} 90 & 4 \\ 1 & 1 \end{pmatrix}$$

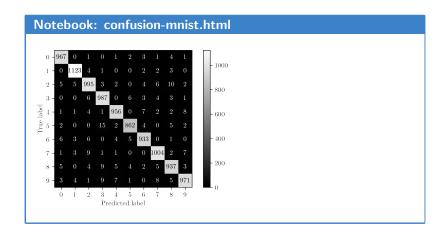
```
Precision = \frac{90}{94}

Recall = \frac{90}{91}

F-Score = 0.9524

Matthew's Coeff. = 0.14
```

Confusion Matrix for multi-class classification



Regression Metrics

Quick Question!

Why might Mean Absolute Error (MAE) be preferred over Mean Squared Error (MSE)?

• a) MAE is always smaller

Quick Question!

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Answer: b) MAE is less sensitive to outliers since it doesn't square the errors!

Metrics for Regression: MSE & MAE

Prediction
$$(\hat{y})$$
 Ground Truth (\mathbf{y})

$$\begin{pmatrix}
10 & & & \\
20 & & & \\
30 & & & \\
40 & & & \\
50 & & & \\
60 & & & \\
\end{pmatrix}$$

Mean Squared Error (MSE) =
$$\frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2}{n}$$
Root Mean Square Error (RMSE) = $\sqrt{\text{MSE}}$

Accuracy Metrics: MAE & ME

Prediction
$$(\hat{y})$$
 Ground Truth

 $\begin{pmatrix}
10 \\
20 \\
30 \\
40 \\
50
\end{pmatrix}$
Ground Truth

 $\begin{pmatrix}
60 \\
60 \\
60
\end{pmatrix}$

Mean Absolute Error (MAE) =
$$\frac{\sum_{i=1}^{n} |\hat{y}_i - y_i|}{n}$$
Mean Error =
$$\frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)}{n}$$

Accuracy Metrics: MAE & ME

Prediction
$$(\hat{y})$$
 Ground Truth

 $\begin{pmatrix}
10 \\
20 \\
30 \\
40 \\
50
\end{pmatrix}$
Ground Truth

 $\begin{pmatrix}
6 \\
40 \\
50 \\
60
\end{pmatrix}$

Mean Absolute Error (MAE) =
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 Mean Error =
$$\frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)}{n}$$

Is there any downside with using mean error?

Accuracy Metrics: MAE & ME

Prediction
$$(\hat{y})$$
 Ground Truth

 $\begin{pmatrix}
10 \\
20 \\
30 \\
40 \\
50
\end{pmatrix}$
Ground Truth

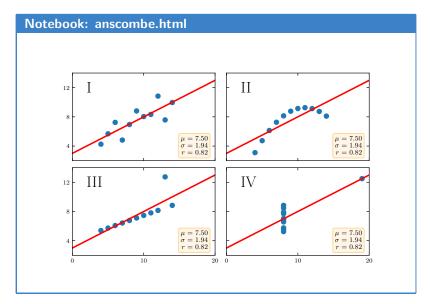
 $\begin{pmatrix}
60 \\
60 \\
60
\end{pmatrix}$

Mean Absolute Error (MAE) =
$$\frac{\sum_{i=1}^{n} |\hat{y}_i - y_i|}{n}$$
Mean Error =
$$\frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)}{n}$$

Is there any downside with using mean error? Errors can get cancelled out

Data Visualization and Baselines

The Importance of Plotting



Dummy Baselines

Notebook: dummy-baselines.html

The Importance of Plotting

Property	Value	Across datasets
mean(X)	9	exact
mean(Y)	7.5	up to 3 decimal places
Linear regression line	y = 3.00 + 0.500x	up to 2 decimal places

Summary and Key Takeaways

Final Challenge!

For imbalanced datasets, which metrics should you prioritize over accuracy?

• a) Only precision

Final Challenge!

- a) Only precision
- b) Only recall

Final Challenge!

- a) Only precision
- b) Only recall
- c) Precision, recall, and F1-score

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Final Challenge!

For imbalanced datasets, which metrics should you prioritize over accuracy?

- a) Only precision
- b) Only recall
- c) Precision, recall, and F1-score
- d) Only confusion matrix

Answer: c) Precision, recall, and F1-score give a more complete picture!

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- Accuracy isn't everything: For imbalanced data, use precision, recall, F1-score
- Visualization is crucial: Always plot your data (Anscombe's Quartet lesson)
- Use baselines: Simple baseline models help validate your approach

Summary: Evaluation Metrics

Task	Common Metrics	When to Use
Classification	Accuracy, Precision, Recall, F1	Balanced/Imbalanced
	Confusion Matrix	Multi-class problems
Regression	MSE, RMSE, MAE	Continuous prediction
	Mean Error	Check for bias

Remember: Choose metrics based on your problem's characteristics and business requirements!